The Analysis of Self-diffusion and Migration of Spheres in Nonlinear Shear Flow Using a Traction-corrected Boundary Element Method

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The goal of this research is to develop an innovative numerical simulation capability for the flow of suspensions of particles in liquids, which is relevant to several important energy-related technologies. We will incorporate effects that span time and length scales associated with molecular to macroscopic phenomena. As part of this goal, at the macroscopic scale, we need to determine how to efficiently model suspensions in situations in which the molecular-scale effects do not dominate, and to determine the limits of applicability of these models. We have developed a traction-corrected boundary element method (TC-BEM) that couples macroscale hydrodynamic forces with fine-scale physicals between particles. We have shown that the TC-BEM is extremely accurate in predicting particle trajectories and can be used to calculate both particle self-diffusivity and newly defined migrations diffusivity for dilute suspensions. This work focuses on development of robust numerical simulation capabilities for suspensions of small solid particles in liquids, incorporating effects spanning diverse time and length scales. In the current research, a new method is developed to incorporate the near-field effects into the boundary element method. Rather than working with lubrication forces as was done previously [1-4], asymptotic solutions have been derived for traction fields in the interstitial regions between particles. The calculation of the traction unknowns, for a single boundary element centered around the point of nearest contact, is based on the relative motion of the two particles in terms of the asymptotic traction solutions. In this way, the system remains fully coupled, incorporating both the boundary element representation for all other elements along with the near-field asymptotics.

As shown in Fig. 1, by combining theoretical analysis with hydrodynamic simulations, TC-BEM is able to correctly model both the far-field macroscale interactions and the near-contact microscale interactions. Using this new tool, we obtained the quantitative agreement of the self-diffusivities with the analytic model [5] for two rough spheres.

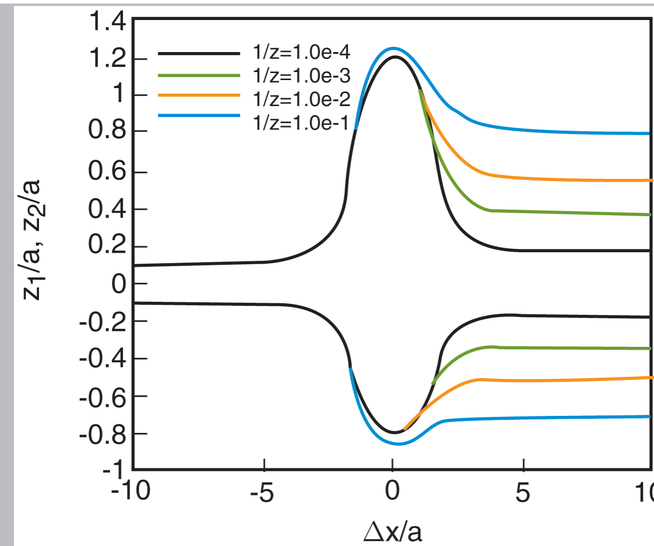

Fig. 1. TC-BEM simulated trajectories in the shear plane of two rough spheres suspended in a nonlinear shear flow.

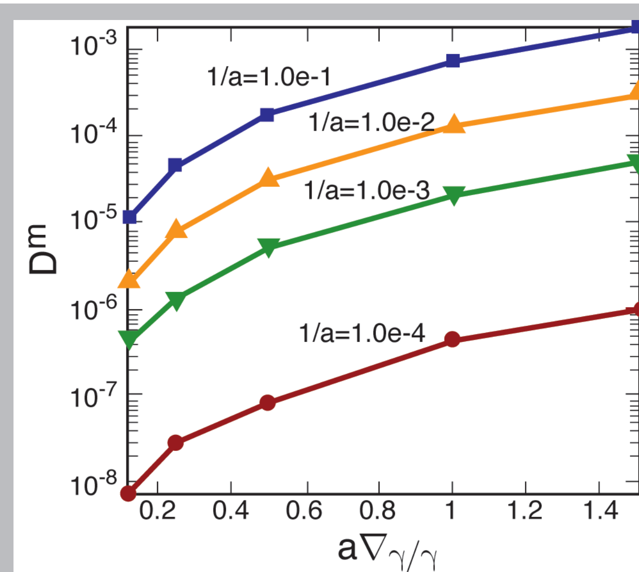

Fig. 2. Migration diffusivity is a strong function of nonlinearity parameter.

The main result of the current study is that there is a net migration of the center of gravity of a pair of rough spheres suspended in a nonlinear shear flow towards the low-shear-rate region of the flow. This migration increases with the nonlinearity of the flow field and with particle roughness as shown in Fig. 2. This new theory was facilitated by our scale-coupling methodology and accurately predicted migration over a range of particle diameter from 0.1 to 3.175 mm.

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